A THREE-DIMENSIONAL FINITE DIFFERENCE TIME DOMAIN - PERFECTLY MATCHED LAYER ALGORITHM BASED ON PIECEWISE-LINEAR APPROXIMATION FOR LINEAR DISPERSIVE MEDIA

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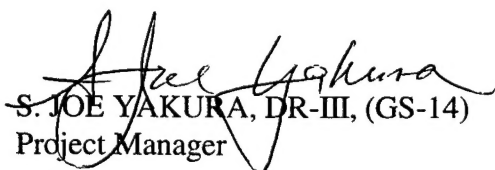
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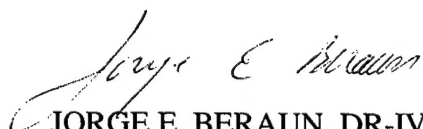
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Abstract

Starting with the unsplit-field uniaxial PML formulation, a second-order accurate FDTD-PML algorithm is obtained using the piecewise-linear approximation. Use of the FDTD-PML algorithm results in the proper long time limit behavior where the electric field value decrease exponentially to zero inside a PML medium long after an electromagnetic pulse is incident on the PML medium. The behavior is consistent with the other PML algorithm, such as Gedney's two-step approach.

I. INTRODUCTION

With the advent of high power computers that provide fast execution times and great quantities of computer memory, we are at the stage where we can perform direct numerical calculations of Maxwell's equations. Out of many numerical techniques available in the computational electromagnetic community, one that has shown a great promise in the time domain is the well-known finite-difference time-domain (FDTD) method [1]. It is based on using a simple staggered differencing scheme in both time and space to calculate the transient behavior of electromagnetic field quantities. One of the greatest challenges of the FDTD methods has been the efficient and accurate formulation of electromagnetic wave interactions in unbounded regions. For such problems, an absorbing boundary condition must be introduced at the outer layer boundary to simulate the extension of the lattice to infinity. One approach that has given a great promise in realizing such an absorbing outer boundary inside the finite volume computational domain is the well-known perfectly-matched-layer (PML) algorithm that was first introduced by J. P. Berenger [2] in 1994 for the free space boundary interface. Since that time Chew and Weedon [3] came up with the modified PML algorithm that is based on complex coordinate stretching, which is shown to be equivalent to the anistropic PML medium approach [4].

In this paper, we explore the formulation of a 3-dimensional PML algorithm used in outer layer absorbing boundary of a dispersive medium to absorb all outgoing waves out of a finite simulation volume. We consider the case where a plane wave propagates outwardly from a dispersive medium to the dispersive PML medium through a reflectionless PML interface. We start the analysis based on unsplit-field uniaxial PML formulation [4-8] of Maxwell's equations that are obtained in the frequency domain inside the dispersive PML medium. We perform the inverse Fourier transform of these equations from the frequency domain to the time domain to obtain a set of ordinary first-order differential equations. Then, these equations are finite differenced in both time and space using the usual Yee FDTD scheme while expanding the electric and magnetic field vectors in time using the Taylor series expansion about the current time step in order to evaluate next time step values of the electromagnetic field quantities. Depending on the number of terms kept in the Taylor series expansion, we can numerically evaluate the updated values to any desired accuracy we want. In Section II, we use the piecewise-linear approximation, which is equivalent to using only the first-order, time-dependent term of the Taylor series expansion, to show the process involved in obtaining a second-order accurate FDTD-PML algorithm. To obtain higher-order accurate FDTD-PML algorithms in time, we simply need to include higher-order, time-dependent terms in the Taylor series expansion and follow the same steps shown in Section II. A consequence of the higher-order accurate FDTD-PML algorithm is the need to solve for zeroes of the nth degree polynomials at each time step in order to update field values. It arises because of the use of the nth-order, time-dependent term of the Taylor series expansion. The numerical process involved in updating the field values is similar to the FDTD algorithm obtained for nonlinear dispersive media [9,10].

II. PML FORMULATION FOR LINEAR DISPERSIVE MEDIA

For a wave propagating into anisotropic, uniaxial dispersive PML media, the modified Maxwell's equations under the PML formulation with stretched coordinates [3] can be expressed in the frequency domain ($e^{i\omega t}$ convention) as

$$\underline{\nabla} \times \underline{E}(\omega; \underline{x}) = -i\omega \, \underline{\underline{S}}^{PML}(\omega) \bullet \mu_0 \mu_R \, \underline{H}(\omega; \underline{x}) , \tag{2.1}$$

$$\underline{\nabla} \times \underline{H}(\omega; \underline{x}) = i\omega \, \underline{\underline{S}}^{PML}(\omega) \bullet \underline{D}(\omega; \underline{x}) , \tag{2.2}$$

with

$$\underline{D}(\omega; \underline{x}) = \varepsilon_0 \varepsilon_R \underline{E}(\omega; \underline{x}) + \varepsilon_0 \sum_{\rho=1}^{\rho_{max}} \underline{P}_\rho(\omega; \underline{x}) , \tag{2.3}$$

$$\underline{P}_\rho(\omega; \underline{x}) = X_\rho^{(1)}(\omega) \, \underline{E}(\omega; \underline{x}) , \tag{2.4}$$

where $\underline{E}(\omega;x)$ is the electric field vector, $\underline{H}(\omega;\underline{x})$ is the magnetic field vector, $\underline{D}(\omega;\underline{x})$ is the displacement field vector, $\underline{P}_\rho(\omega;\underline{x})$ is the electric polarization vector, $\underline{\underline{S}}^{PML}(\omega)$ is the uniaxial anisotropic PML matrix, ε_0 is the free space electric permittivity, ε_R is the relative permittivity, μ_0 is the free-space permeability, μ_R is the relative permeability, and $X_\rho^{(1)}(\omega)$ is the ρth term of the collection consisting of ρ_{max} frequency-dependent, first-order (linear) electric susceptibility functions, where ρ_{max} is the maximum number of terms which we choose to consider for a particular formulation of Eq. (2.3). Also seen in the above equations is the notation $\bullet$ that is used to denote a dot product. Elements of the uniaxial anisotropic PML matrix, $\underline{\underline{S}}^{PML}(\omega)$, are given by

$$\underline{\underline{S}}^{PML}(\omega) = \begin{pmatrix} \dfrac{S_y(\omega) S_z(\omega)}{S_x(\omega)} & 0 & 0 \\[2ex] 0 & \dfrac{S_x(\omega) S_z(\omega)}{S_y(\omega)} & 0 \\[2ex] 0 & 0 & \dfrac{S_x(\omega) S_y(\omega)}{S_z(\omega)} \end{pmatrix} , \tag{2.5}$$

where $S_x(\omega)$, $S_y(\omega)$ and $S_z(\omega)$ are arbitrarily defined ω-dependent functions that satisfy the impedance matching condition at the interface of the non-PML medium and the PML medium. It is a common practice in the FDTD community to choose $S_x(\omega)$, $S_y(\omega)$ and $S_z(\omega)$ in the following forms:

$$S_x(\omega) = 1 + \frac{\sigma_x}{i\omega\varepsilon_0\varepsilon_R} \quad \text{with} \quad \frac{\sigma_x}{\varepsilon_0\varepsilon_R} = \frac{\sigma_x^*}{\mu_0\mu_R} , \tag{2.6-2.7}$$

$$S_y(\omega) = 1 + \frac{\sigma_y}{i\omega\varepsilon_0\varepsilon_R} \quad \text{with} \quad \frac{\sigma_y}{\varepsilon_0\varepsilon_R} = \frac{\sigma_y^*}{\mu_0\mu_R} , \text{ and} \tag{2.8-2.9}$$

$$S_z(\omega) = 1 + \frac{\sigma_z}{i\omega\varepsilon_0\varepsilon_R} \quad \text{with} \quad \frac{\sigma_z}{\varepsilon_0\varepsilon_R} = \frac{\sigma_z^*}{\mu_0\mu_R} , \tag{2.10-2.11}$$

where σ_x, σ_y and σ_z are the PML electric conductivities, and σ_x^*, σ_y^* and σ_z^* are the PML magnetic conductivities with subscripts x, y and z denoting the directions in which PML conductivities are assigned [2]. These PML conductivities are introduced arbitrarily in order to implement the FDTD-PML algorithm.

We first eliminate $\underline{D}(\omega;\underline{x})$ in favor of expressing Maxwell's equations in terms of $\underline{E}(\omega;\underline{x})$ and $\underline{P}_\rho(\omega;\underline{x})$ by substituting Eq. (2.3) into Eq. (2.2). Upon taking the inverse Fourier transforms of Eqs. (2.1), (2.2) and (2.4) and using the expressions shown in Eqs. (2.6) through (2.11), we can show after some manipulations Eqs. (2.1), (2.2) and (2.4) are written in the following time-dependent equations:

$$\mu_0\mu_R\frac{\partial \underline{H}(t;\underline{x})}{\partial t}+\mu_0\mu_R\underline{\underline{\Psi}}_0\bullet\underline{H}(t;\underline{x})+\mu_0\mu_R\underline{\underline{\Psi}}_1\bullet\underline{H}^{Delay}(t;\underline{x})+\underline{\nabla}\times\underline{E}(t;\underline{x})=0\,,\tag{2.12}$$

$$\varepsilon_0\varepsilon_R\frac{\partial \underline{E}(t;\underline{x})}{\partial t}+\varepsilon_0\sum_\rho\frac{\partial \underline{P}_\rho(t;\underline{x})}{\partial t}+\varepsilon_0\underline{\underline{\Psi}}_0\bullet\left[\varepsilon_R\underline{E}(t;\underline{x})+\sum_\rho\underline{P}_\rho(t;\underline{x})\right]$$
$$+\varepsilon_0\underline{\underline{\Psi}}_1\bullet\left[\varepsilon_R\underline{E}^{Delay}(t;\underline{x})+\sum_\rho\underline{P}_\rho^{Delay}(t;\underline{x})\right]-\underline{\nabla}\times\underline{H}(t;\underline{x})=0\,,\tag{2.13}$$

with

$$\underline{P}_\rho(t;\underline{x})=\int_{-\infty}^{\infty}d\tau\,X_\rho^{(1)}(t-\tau)\,\underline{E}(\tau;\underline{x})\,,\tag{2.14}$$

$$\underline{H}^{Delay}(t;\underline{x})=\int_{-\infty}^{t}d\tau\,\underline{\underline{\Phi}}(t-\tau)\bullet\underline{H}(\tau;\underline{x})\,,\tag{2.15}$$

$$\underline{E}^{Delay}(t;\underline{x})=\int_{-\infty}^{t}d\tau\,\underline{\underline{\Phi}}(t-\tau)\bullet\underline{E}(\tau;\underline{x})\,,\tag{2.16}$$

$$\underline{P}_\rho^{Delay}(t;\underline{x})=\int_{-\infty}^{t}d\tau\,\underline{\underline{\Phi}}(t-\tau)\bullet\underline{P}_\rho(\tau;\underline{x})\,,\tag{2.17}$$

where

$$\underline{\underline{\Psi}}_0=\begin{pmatrix}\left(\dfrac{\sigma_y}{\varepsilon_0\varepsilon_R}+\dfrac{\sigma_z}{\varepsilon_0\varepsilon_R}-\dfrac{\sigma_x}{\varepsilon_0\varepsilon_R}\right) & 0 & 0 \\[2mm] 0 & \left(\dfrac{\sigma_x}{\varepsilon_0\varepsilon_R}+\dfrac{\sigma_z}{\varepsilon_0\varepsilon_R}-\dfrac{\sigma_y}{\varepsilon_0\varepsilon_R}\right) & 0 \\[2mm] 0 & 0 & \left(\dfrac{\sigma_x}{\varepsilon_0\varepsilon_R}+\dfrac{\sigma_y}{\varepsilon_0\varepsilon_R}-\dfrac{\sigma_z}{\varepsilon_0\varepsilon_R}\right)\end{pmatrix}\,,\tag{2.18}$$

$$\underline{\underline{\Psi}}_1=\begin{pmatrix}\left(\dfrac{\sigma_y}{\varepsilon_0\varepsilon_R}-\dfrac{\sigma_x}{\varepsilon_0\varepsilon_R}\right)\left(\dfrac{\sigma_z}{\varepsilon_0\varepsilon_R}-\dfrac{\sigma_x}{\varepsilon_0\varepsilon_R}\right) & 0 & 0 \\[2mm] 0 & \left(\dfrac{\sigma_x}{\varepsilon_0\varepsilon_R}-\dfrac{\sigma_y}{\varepsilon_0\varepsilon_R}\right)\left(\dfrac{\sigma_z}{\varepsilon_0\varepsilon_R}-\dfrac{\sigma_y}{\varepsilon_0\varepsilon_R}\right) & 0 \\[2mm] 0 & 0 & \left(\dfrac{\sigma_x}{\varepsilon_0\varepsilon_R}-\dfrac{\sigma_z}{\varepsilon_0\varepsilon_R}\right)\left(\dfrac{\sigma_y}{\varepsilon_0\varepsilon_R}-\dfrac{\sigma_z}{\varepsilon_0\varepsilon_R}\right)\end{pmatrix}\,,\tag{2.19}$$

$$\underline{\underline{\Phi}}(t-\tau)=\begin{pmatrix}\exp[-(\dfrac{\sigma_x}{\varepsilon_0\varepsilon_R})(t-\tau)] & 0 & 0 \\[2mm] 0 & \exp[-(\dfrac{\sigma_y}{\varepsilon_0\varepsilon_R})(t-\tau)] & 0 \\[2mm] 0 & 0 & \exp[-(\dfrac{\sigma_z}{\varepsilon_0\varepsilon_R})(t-\tau)]\end{pmatrix}\,.\tag{2.20}$$

In the above, $\underline{H}^{Delay}(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$ and $\underline{P}_\rho^{Delay}(t;\underline{x})$ are introduced to handle the delayed time-response behavior of $\underline{H}(t;\underline{x})$, $\underline{E}(t;\underline{x})$ and $\underline{P}_\rho(t;\underline{x})$, respectively. These functions follow naturally from taking the inverse Fourier transforms of convolution functions $[1/(i\omega\underline{\underline{I}}+\underline{\underline{A}})]\underline{H}(\omega;\underline{x})$, $[1/(i\omega\underline{\underline{I}}+\underline{\underline{A}})]\underline{E}(\omega;\underline{x})$, and $[1/(i\omega\underline{\underline{I}}+\underline{\underline{A}})]\underline{P}_\rho(\omega;\underline{x})$ by realizing the inverse Fourier transform of $[1/(i\omega\underline{\underline{I}}+\underline{\underline{A}})]$ is given by $\exp(-\underline{\underline{A}}t)$, where $\underline{\underline{A}}$ is a time independent diagonal matrix expressed as diag$[\sigma_x/(\varepsilon_0\varepsilon_R),\sigma_y/(\varepsilon_0\varepsilon_R),\sigma_z/(\varepsilon_0\varepsilon_R)]$.

To solve Eqs. (2.12), (2.13), (2.14), (2.15), (2.16) and (2.17), we need to specify the expression for the linear electric susceptibility function. In this paper we consider the case in which the linear electric

susceptibility function is expressed as a complex function that contains complex constant coefficients and exhibit exponential behavior in the time domain as follows:

$$X_\rho^{(1)}(t) = \mathrm{Re}\left\{\alpha_\rho \exp[-(\gamma_\rho)t]\right\} U(t), \tag{2.21}$$

where Re{ } is used to represent the real part of a complex function, $U(t)$ is the unit step function, and α_ρ and γ_ρ are complex constant coefficients. Now, Eq. (2.14) takes the form

$$\underline{P}_\rho(t;\underline{x}) \equiv \mathrm{Re}\left\{\underline{Q}_\rho(t;\underline{x})\right\} = \mathrm{Re}\left\{\alpha_\rho \int_{-\infty}^{t} d\tau \exp[-(\gamma_\rho)(t-\tau)]\,\underline{E}(\tau;\underline{x})\right\}, \tag{2.22}$$

where complex function $\underline{Q}_\rho(t;\underline{x})$ is introduced in the above equation such that the real part of the complex function results in $\underline{P}_\rho(t;\underline{x})$.

We need to point out that by making the proper choices of complex constant coefficients and performing the Fourier transform of Eq. (2.21), we can readily obtain the familiar constant conductivity [i.e., α_ρ is real and $\gamma_\rho = 0$], Debye [i.e., α_ρ and γ_ρ are both real] and Lorentz [i.e., α_ρ is imaginary and γ_ρ is real] forms of the complex permittivity in the frequency domain.

To derive FDTD expressions based on Yee FDTD scheme, Eqs. (2.12), (2.13), (2.14), (2.15), (2.16) and (2.17) have to be solved numerically for $\underline{H}(t;\underline{x})$, $\underline{E}(t;\underline{x})$, $\underline{P}_\rho(t;\underline{x})$, $\underline{H}^{Delay}(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$ and $\underline{P}_\rho^{Delay}(t;\underline{x})$ at each time step by correctly carrying out the numerical integration of convolution integrals $\underline{P}_\rho(t;\underline{x})$, $\underline{H}^{Delay}(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$ and $\underline{P}_\rho^{Delay}(t;\underline{x})$. Therefore, the whole solution rests on the question of how to carry out the numerical integration of $\underline{P}_\rho(t;\underline{x})$, $\underline{H}^{Delay}(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$ and $\underline{P}_\rho^{Delay}(t;\underline{x})$ at each successive time step. For that reason, the rest of this section is devoted to the numerical formulation that treats $\underline{P}_\rho(t;\underline{x})$, $\underline{H}^{Delay}(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$ and $\underline{P}_\rho^{Delay}(t;\underline{x})$ into the overall FDTD scheme based on the recursive convolution approach.

We first convert the convolution integrals $\underline{P}_\rho(t;\underline{x})$, $\underline{H}^{Delay}(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$ and $\underline{P}_\rho^{Delay}(t;\underline{x})$ [i.e., Eqs. (2.22), (2.15), (2.16) and (2.17)] into the following equivalent first-order differential equations:

$$\frac{\partial \underline{Q}_\rho(t;\underline{x})}{\partial t} + (\gamma_\rho)\underline{Q}_\rho(t;\underline{x}) = \alpha_\rho \underline{E}(t;\underline{x}), \tag{2.23}$$

$$\frac{\partial \underline{H}^{Delay}(t;\underline{x})}{\partial t} + \underline{\underline{\Phi}}(t) \bullet \underline{H}^{Delay}(t;\underline{x}) = \underline{H}(t;\underline{x}), \tag{2.24}$$

$$\frac{\partial \underline{E}^{Delay}(t;\underline{x})}{\partial t} + \underline{\underline{\Phi}}(t) \bullet \underline{E}^{Delay}(t;\underline{x}) = \underline{E}(t;\underline{x}), \tag{2.25}$$

$$\frac{\partial \underline{Q}_\rho^{Delay}(t;\underline{x})}{\partial t} + \underline{\underline{\Phi}}(t) \bullet \underline{Q}_\rho^{Delay}(t;\underline{x}) = \underline{Q}_\rho(t;\underline{x}), \tag{2.26}$$

where complex function $\underline{Q}_\rho^{Delay}(t;\underline{x})$ is introduced in Eq. (2.26) such that the real part of the complex function results in $\underline{P}_\rho^{Delay}(t;\underline{x})$.

To show how we can use Eqs. (2.12), (2.13), (2.23), (2.24), (2.25) and (2.26) to come up with a 3-D FDTD-PML algorithm for dispersive PML media, we integrate Eqs. (2.12) and (2.24) from $t=(n-\frac{1}{2})\Delta t$ to $t=(n+\frac{1}{2})\Delta t$, and Eqs. (2.13), (2.23), (2.25) and (2.26) from $t=n\Delta t$ to $t=(n+1)\Delta t$. Then Eqs. (2.23), (2.24), (2.25) and (2.26) are solved exactly using the integrating factor technique for a given discrete time interval to go forward in time by Δt. The result is that we need to evaluate definite integrals appearing in the following equations:

$$\mu_0\mu_R \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \frac{\partial \underline{H}(\tau;\underline{x})}{\partial \tau} + \mu_0\mu_R \underline{\underline{\Psi}}_0 \bullet \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau\, \underline{H}(\tau;\underline{x})$$

$$+ \mu_0\mu_R \underline{\underline{\Psi}}_1 \bullet \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau\, \underline{H}^{Delay}(\tau;\underline{x}) + \int_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau\, \underline{\nabla} \times \underline{E}(\tau;\underline{x}) = 0, \tag{2.27}$$

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$$\varepsilon_0\varepsilon_R \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau \frac{\partial \underline{E}(\tau;\underline{x})}{\partial \tau} + \varepsilon_0 \operatorname{Re}\{\sum_\rho \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau \frac{\partial \underline{Q}_\rho(\tau;\underline{x})}{\partial \tau}\}$$

$$+ \varepsilon_0\varepsilon_R \underline{\underline{\Psi}}_0 \bullet \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau\, \underline{E}(\tau;\underline{x}) + \varepsilon_0 \underline{\underline{\Psi}}_0 \bullet \operatorname{Re}\{\sum_\rho \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau\, \underline{Q}_\rho(\tau;\underline{x})\}$$

$$+ \varepsilon_0\varepsilon_R \underline{\underline{\Psi}}_1 \bullet \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau\, \underline{E}^{\text{Delay}}(\tau;\underline{x}) + \varepsilon_0 \underline{\underline{\Psi}}_1 \bullet \operatorname{Re}\{\sum_\rho \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau\, \underline{Q}_\rho^{\text{Delay}}(\tau;\underline{x})\}$$

$$- \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau\, \underline{\nabla} \times \underline{H}(\tau;\underline{x}) = 0, \tag{2.28}$$

$$\underline{Q}_\rho(n\Delta t + \Delta t;\underline{x}) = \exp[-(\gamma_\rho)\Delta t]\big[\underline{Q}_\rho(n\Delta t;\underline{x}) + \alpha_\rho \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-(\gamma_\rho)(n\Delta t - \tau)]\underline{E}(\tau;\underline{x})\big], \tag{2.29}$$

$$\underline{H}^{\text{Delay}}(n\Delta t + \tfrac{1}{2}\Delta t;\underline{x}) = \exp(-\underline{\underline{\Phi}}\Delta t) \bullet \big[\underline{H}^{\text{Delay}}(n\Delta t - \tfrac{1}{2}\Delta t;\underline{x})$$

$$+ \int\limits_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \exp[-\underline{\underline{\Phi}}(n\Delta t - \tfrac{1}{2}\Delta t - \tau)] \bullet \underline{H}(\tau;\underline{x})\big], \tag{2.30}$$

$$\underline{E}^{\text{Delay}}(n\Delta t + \Delta t;\underline{x}) = \exp(-\underline{\underline{\Phi}}\Delta t) \bullet \big[\underline{E}^{\text{Delay}}(n\Delta t;\underline{x}) + \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-\underline{\underline{\Phi}}(n\Delta t - \tau)] \bullet \underline{E}(\tau;\underline{x})\big], \tag{2.31}$$

$$\underline{Q}_\rho^{\text{Delay}}(n\Delta t + \Delta t;\underline{x}) = \exp(-\underline{\underline{\Phi}}\Delta t) \bullet \big[\underline{Q}_\rho^{\text{Delay}}(n\Delta t;\underline{x}) + \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-\underline{\underline{\Phi}}(n\Delta t - \tau)] \bullet \underline{Q}_\rho(\tau;\underline{x})\big]$$

$$= \exp(-\underline{\underline{\Phi}}\Delta t) \bullet \big[Q_\rho^{\text{Delay}}(n\Delta t;\underline{x}) + \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-\underline{\underline{\Phi}}(n\Delta t - \tau) - \underline{\underline{I}}(\gamma_\rho)(\tau - n\Delta t)] \bullet \underline{Q}_\rho(n\Delta t;\underline{x})$$

$$+ \alpha_\rho \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau \int\limits_{n\Delta t}^{\tau} d\tau' \exp[-\underline{\underline{\Phi}}(n\Delta t - \tau) - \underline{\underline{I}}(\gamma_\rho)(\tau - \tau')] \bullet \underline{E}(\tau';\underline{x})\big], \tag{2.32}$$

where $\underline{\underline{I}}$ is the identity matrix. Furthermore, some of those definite integrals that appear in Eqs. (2.27) and (2.28) are manipulated and cast in the following forms:

$$\int\limits_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau\, \underline{H}^{\text{Delay}}(\tau;\underline{x}) = \int\limits_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \exp[-\underline{\underline{\Phi}}(\tau - n\Delta t + \tfrac{1}{2}\Delta t)] \bullet \underline{H}^{\text{Delay}}(n\Delta t - \tfrac{1}{2}\Delta t;\underline{x})$$

$$+ \int\limits_{(n-\frac{1}{2})\Delta t}^{(n+\frac{1}{2})\Delta t} d\tau \int\limits_{(n-\frac{1}{2})\Delta t}^{\tau} d\tau' \exp[-\underline{\underline{\Phi}}(\tau - \tau')] \bullet \underline{H}(\tau';\underline{x}), \tag{2.33}$$

$$\int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau\, \underline{Q}_\rho(\tau;\underline{x}) = \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau \exp[-(\gamma_\rho)(\tau - n\Delta t)] \underline{Q}_\rho(n\Delta t;\underline{x})$$

$$+ \alpha_\rho \int\limits_{n\Delta t}^{(n+1)\Delta t} d\tau \int\limits_{n\Delta t}^{\tau} d\tau' \exp[-(\gamma_\rho)(\tau - \tau')] \underline{E}(\tau';\underline{x}), \tag{2.34}$$

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$$\int_{n\Delta t}^{(n+1)\Delta t} d\tau\, \underline{E}^{Delay}(\tau;\underline{x}) = \int_{n\Delta t}^{(n+1)\Delta t} d\tau\, \exp[-\underline{\underline{\Phi}}\,(\tau-n\Delta t)]\bullet \underline{E}^{Delay}(n\Delta t;\underline{x})$$

$$+ \int_{n\Delta t}^{(n+1)\Delta t} d\tau \int_{n\Delta t}^{\tau} d\tau'\exp[-\underline{\underline{\Phi}}(\tau-\tau')]\bullet \underline{E}(\tau';\underline{x}),\qquad(2.35)$$

$$\int_{n\Delta t}^{(n+1)\Delta t} d\tau\, \underline{Q}_\rho^{Delay}(\tau;\underline{x}) = \int_{n\Delta t}^{(n+1)\Delta t} d\tau\, \exp[-\underline{\underline{\Phi}}\,(\tau-n\Delta t)]\bullet \underline{Q}_\rho^{Delay}(n\Delta t;\underline{x})$$

$$+ \int_{n\Delta t}^{(n+1)\Delta t} d\tau \int_{n\Delta t}^{\tau} d\tau'\exp[-\underline{\underline{\Phi}}\,\tau - \underline{\underline{I}}\,(\gamma_\rho)(\tau'-n\Delta t)]\bullet \underline{Q}_\rho(n\Delta t;\underline{x})$$

$$+\alpha_\rho \int_{n\Delta t}^{(n+1)\Delta t} d\tau \int_{n\Delta t}^{\tau} d\tau' \int_{n\Delta t}^{\tau'} d\tau''\exp[-\underline{\underline{\Phi}}\,\tau - \underline{\underline{I}}\,(\gamma_\rho)(\tau'-\tau'')]\bullet \underline{E}(\tau'';\underline{x}).\qquad(2.36)$$

To obtain second-order accuracy in time from a finite differencing technique, $\underline{H}(t;\underline{x})$ and $\underline{E}(t;\underline{x})$ are taken to be piecewise-linear continuous functions over the entire temporal integration range such that $\underline{H}(t;\underline{x})$ and $\underline{E}(t;\underline{x})$ change linearly with respect to time over given discrete time step intervals. It is equivalent to using only the first-order, time-dependent terms of the Taylor series expansions for $\underline{H}(t;\underline{x})$ and $\underline{E}(t;\underline{x})$, respectively, expanded in time about current time step of $\underline{H}(t;\underline{x})$ and $\underline{E}(t;\underline{x})$. Mathematically, we can express $\underline{H}(t;\underline{x})$ and $\underline{E}(t;\underline{x})$ in the following forms in terms of $(\underline{H})_{ijk}^{n-\frac{1}{2}}$, $(\underline{H})_{ijk}^{n+\frac{1}{2}}$, $(\underline{E})_{ijk}^{n}$ and $(\underline{E})_{ijk}^{n+1}$ where superscripts $n-\frac{1}{2}$, n, $n+\frac{1}{2}$ and $n+1$ are used to denote discrete time steps at $t=(n-\frac{1}{2})\Delta t$, $t=n\Delta t$, $t=(n+\frac{1}{2})\Delta t$ and $t=(n+1)\Delta t$, respectively. Subscripts are used to denote discrete spatial locations, $\underline{x}=[i\Delta x, j\Delta y, k\Delta z]$ for $\underline{E}(t;\underline{x})$ and $\underline{x}=[(i-\frac{1}{2})\Delta x, (j-\frac{1}{2})\Delta y, (k-\frac{1}{2})\Delta z]$ for $\underline{H}(t;\underline{x})$, with Δx, Δy and Δz being the spatial grid sizes in the x, y and z directions, respectively.

$$\underline{H}(t;\underline{x}) = \begin{cases} (\underline{H})_{ijk}^{n-\frac{1}{2}} + \dfrac{[(\underline{H})_{ijk}^{n+\frac{1}{2}} - (\underline{H})_{ijk}^{n-\frac{1}{2}}]}{\Delta t}[t-(n-\frac{1}{2})\Delta t] + \text{higher order terms,} \\[1em] \qquad\qquad\qquad\qquad\qquad \text{for}\quad 0 \le (n-\frac{1}{2})\Delta t \le t \le (n+\frac{1}{2})\Delta t \qquad(2.37) \\[1em] 0, \qquad\qquad\qquad\qquad\qquad\qquad \text{for}\quad t < 0 \end{cases}$$

$$\underline{E}(t;\underline{x}) = \begin{cases} (\underline{E})_{ijk}^{n} + \dfrac{[(\underline{E})_{ijk}^{n+1} - (\underline{E})_{ijk}^{n}]}{\Delta t}(t-n\Delta t) + \text{higher order terms,} \\[1em] \qquad\qquad\qquad\qquad\qquad \text{for}\quad 0 \le n\Delta t \le t \le (n+1)\Delta t \qquad(2.38) \\[1em] 0, \qquad\qquad\qquad\qquad\qquad\qquad \text{for}\quad t < 0 \end{cases}$$

By keeping more than the first-order, time-dependent term in the above Taylor series expansion, it is possible to investigate higher than second-order accurate FDTD algorithms.

Substituting Eqs. (2.37) and (2.38) into Eqs. (2.27) through (2.36), performing the time integration from $t=(n-\frac{1}{2})\Delta t$ to $t=(n+\frac{1}{2})\Delta t$ for field values that depend on the magnetic field [i.e., $\underline{H}(t;\underline{x})$ and $\underline{H}^{Delay}(t;\underline{x})$], and from $t=n\Delta t$ to $t=(n+1)\Delta t$ for field values that depend on the electric field [i.e., $\underline{E}(t;\underline{x})$, $\underline{Q}_\rho(t;\underline{x})$, $\underline{E}^{Delay}(t;\underline{x})$ and $\underline{Q}_\rho^{Delay}(t;\underline{x})$] and using the usual staggered Yee FDTD scheme for spatial discretization, we obtain a 3-dimensional FDTD-PML algorithm in Cartesian coordinates. . After some manipulations, we obtain the following six equations which constitute the entire set of updating expressions needed to update field values $(\underline{E})_{ijk}^{n+1}$, $(\underline{H})_{ijk}^{n+1}$, $(\underline{Q}_\rho)_{ijk}^{n+1}$, $(\underline{E}^{Delay})_{ijk}^{n+1}$, $(\underline{H}^{Delay})_{ijk}^{n+1}$ and $(\underline{Q}_\rho^{Delay})_{ijk}^{n+1}$ inside a dispersive PML medium:

$$\underline{\underline{\Omega}}_0 \bullet (\underline{H})_{ijk}^{n+\frac{1}{2}} + \underline{\underline{\Omega}}_1 \bullet (\underline{H})_{ijk}^{n-\frac{1}{2}} + \underline{\underline{\Omega}}_2 \bullet (\underline{H}^{Delay})_{ijk}^{n-\frac{1}{2}} + \underline{S}_E = 0,\qquad(2.39)$$

$$\underline{\underline{\Omega}}_3 \bullet (\underline{E})_{ijk}^{n+1} + \underline{\underline{\Omega}}_4 \bullet (\underline{E})_{ijk}^{n} + \text{Re}\{\sum_{\rho} \underline{\underline{\Gamma}}_{\rho,0} \bullet (\underline{Q}_{\rho})_{ijk}^{n}\}$$

$$+ \underline{\underline{\Omega}}_2 \bullet (\underline{E}^{\text{Delay}})_{ijk}^{n} + \underline{\underline{\Omega}}_5 \bullet \text{Re}\{\sum_{\rho} (\underline{Q}_{\rho}^{\text{Delay}})_{ijk}^{n}\} + \underline{S}_{\text{H}} = 0, \tag{2.40}$$

$$(\underline{Q}_{\rho})_{ijk}^{n+1} = \Theta_{\rho,0}\left[(\underline{Q}_{\rho})_{ijk}^{n} + \Theta_{\rho,1}(\underline{E})_{ijk}^{n} + \Theta_{\rho,2}(\underline{E})_{ijk}^{n+1} \right], \tag{2.41}$$

$$(\underline{H}^{\text{Delay}})_{ijk}^{n+\frac{1}{2}} = \underline{\underline{\Omega}}_6 \bullet \left[(\underline{H}^{\text{Delay}})_{ijk}^{n-\frac{1}{2}} + \underline{\underline{\Omega}}_7 \bullet (\underline{H})_{ijk}^{n-\frac{1}{2}} + \underline{\underline{\Omega}}_8 \bullet (\underline{H})_{ijk}^{n+\frac{1}{2}} \right], \tag{2.42}$$

$$(\underline{E}^{\text{Delay}})_{ijk}^{n+1} = \underline{\underline{\Omega}}_6 \bullet \left[(\underline{E}^{\text{Delay}})_{ijk}^{n} + \underline{\underline{\Omega}}_7 \bullet (\underline{E})_{ijk}^{n} + \underline{\underline{\Omega}}_8 \bullet (\underline{E})_{ijk}^{n+1} \right], \tag{2.43}$$

$$(\underline{Q}_{\rho}^{\text{Delay}})_{ijk}^{n+1} = \underline{\underline{\Omega}}_6 \bullet \left[(\underline{Q}_{\rho}^{\text{Delay}})_{ijk}^{n} + \underline{\underline{\Pi}}_{\rho,0} \bullet (\underline{Q}_{\rho})_{ijk}^{n} + \underline{\underline{\Pi}}_{\rho,1} \bullet (\underline{E})_{ijk}^{n} + \underline{\underline{\Pi}}_{\rho,2} \bullet (\underline{E})_{ijk}^{n+1} \right], \tag{2.44}$$

where $\underline{S}_{\text{E}}$ and $\underline{S}_{\text{H}}$ are given by

$$\underline{S}_{\text{E}} = \begin{pmatrix} \dfrac{\Delta t}{(\mu_0\mu_R)\Delta y}\left[(E_z)_{i(j+\frac{1}{2})k}^{n} - (E_z)_{i(j-\frac{1}{2})k}^{n}\right] - \dfrac{\Delta t}{(\mu_0\mu_R)\Delta z}\left[(E_y)_{ij(k+\frac{1}{2})}^{n} - (E_y)_{ij(k-\frac{1}{2})}^{n}\right] \\ \dfrac{\Delta t}{(\mu_0\mu_R)\Delta z}\left[(E_x)_{ij(k+\frac{1}{2})}^{n} - (E_x)_{ij(k-\frac{1}{2})}^{n}\right] - \dfrac{\Delta t}{(\mu_0\mu_R)\Delta x}\left[(E_z)_{(i+\frac{1}{2})jk}^{n} - (E_z)_{(i-\frac{1}{2})jk}^{n}\right] \\ \dfrac{\Delta t}{(\mu_0\mu_R)\Delta x}\left[(E_y)_{(i+\frac{1}{2})jk}^{n} - (E_y)_{(i-\frac{1}{2})jk}^{n}\right] - \dfrac{\Delta t}{(\mu_0\mu_R)\Delta y}\left[(E_x)_{i(j+\frac{1}{2})k}^{n} - (E_x)_{i(j-\frac{1}{2})k}^{n}\right] \end{pmatrix}, \tag{2.45}$$

$$\underline{S}_{\text{H}} = \begin{pmatrix} -\dfrac{\Delta t}{(\varepsilon_0\varepsilon_R)\Delta y}\left[(H_z)_{i(j+\frac{1}{2})k}^{n+\frac{1}{2}} - (H_z)_{i(j-\frac{1}{2})k}^{n+\frac{1}{2}}\right] + \dfrac{\Delta t}{(\varepsilon_0\varepsilon_R)\Delta z}\left[(H_y)_{ij(k+\frac{1}{2})}^{n+\frac{1}{2}} - (H_y)_{ij(k-\frac{1}{2})}^{n+\frac{1}{2}}\right] \\ -\dfrac{\Delta t}{(\varepsilon_0\varepsilon_R)\Delta z}\left[(H_x)_{ij(k+\frac{1}{2})}^{n+\frac{1}{2}} - (H_x)_{ij(k-\frac{1}{2})}^{n+\frac{1}{2}}\right] + \dfrac{\Delta t}{(\varepsilon_0\varepsilon_R)\Delta x}\left[(H_z)_{(i+\frac{1}{2})jk}^{n+\frac{1}{2}} - (H_z)_{(i-\frac{1}{2})jk}^{n+\frac{1}{2}}\right] \\ -\dfrac{\Delta t}{(\varepsilon_0\varepsilon_R)\Delta x}\left[(H_y)_{(i+\frac{1}{2})jk}^{n+\frac{1}{2}} - (H_y)_{(i-\frac{1}{2})jk}^{n+\frac{1}{2}}\right] + \dfrac{\Delta t}{(\varepsilon_0\varepsilon_R)\Delta y}\left[(H_x)_{i(j+\frac{1}{2})k}^{n+\frac{1}{2}} - (H_x)_{i(j-\frac{1}{2})k}^{n+\frac{1}{2}}\right] \end{pmatrix}, \tag{2.46}$$

and $\Theta_{\rho,0}$, $\Theta_{\rho,1}$ and $\Theta_{\rho,2}$ are the time-invariant coefficients, and $\underline{\underline{\Omega}}_0$, $\underline{\underline{\Omega}}_1$, $\underline{\underline{\Omega}}_2$, $\underline{\underline{\Omega}}_3$, $\underline{\underline{\Omega}}_4$, $\underline{\underline{\Omega}}_5$, $\underline{\underline{\Omega}}_6$, $\underline{\underline{\Omega}}_7$, $\underline{\underline{\Omega}}_8$, $\underline{\underline{\Gamma}}_{\rho,0}$, $\underline{\underline{\Pi}}_{\rho,0}$, $\underline{\underline{\Pi}}_{\rho,1}$ and $\underline{\underline{\Pi}}_{\rho,2}$ are the time-invariant matrices. Both time-invariant coefficients and matrices depend only on material properties α_{ρ}, γ_{ρ}, σ_x, σ_y and σ_z, and time increment Δt. Shown in Appendix A are the explicit expressions of these coefficients and matrices expressed in terms of α_{ρ}, γ_{ρ}, σ_x, σ_y, σ_z and Δt.

Using the above FDTD-PML algorithm the computer simulation can be performed for electromagnetic waves that propagate inside dispersive PML media by simply going through the following steps:

(1) First, before updating the field values, time-invariant coefficients $\Theta_{\rho,0}$, $\Theta_{\rho,1}$ and $\Theta_{\rho,2}$, and time-invariant matrices $\underline{\underline{\Omega}}_0$, $\underline{\underline{\Omega}}_1$, $\underline{\underline{\Omega}}_2$, $\underline{\underline{\Omega}}_3$, $\underline{\underline{\Omega}}_4$, $\underline{\underline{\Omega}}_5$, $\underline{\underline{\Omega}}_6$, $\underline{\underline{\Omega}}_7$, $\underline{\underline{\Omega}}_8$, $\underline{\underline{\Gamma}}_{\rho,0}$, $\underline{\underline{\Pi}}_{\rho,0}$, $\underline{\underline{\Pi}}_{\rho,1}$ and $\underline{\underline{\Pi}}_{\rho,2}$ are calculated at the beginning of the simulation as part of the initial condition for given values of α_{ρ}, γ_{ρ}, σ_x, σ_y, σ_z and Δt. These calculated values are stored in memory and used at each time step to update field values $(\underline{E})_{ijk}^{n+1}$, $(\underline{H})_{ijk}^{n+1}$, $(\underline{Q}_{\rho})_{ijk}^{n+1}$, $(\underline{E}^{\text{Delay}})_{ijk}^{n+1}$, $(\underline{H}^{\text{Delay}})_{ijk}^{n+1}$ and $(\underline{Q}_{\rho}^{\text{Delay}})_{ijk}^{n+1}$.

(2) Using Eq. (2.39), $(\underline{H})_{ijk}^{n+\frac{1}{2}}$ is calculated based on the known values of $(\underline{H})_{ijk}^{n-\frac{1}{2}}$ and $(\underline{H}^{\text{Delay}})_{ijk}^{n-\frac{1}{2}}$ and $(\underline{E})_{ijk}^{n}$.

(3) Using Eq. (2.42), $(\underline{H}^{\text{Delay}})_{ijk}^{n+\frac{1}{2}}$ is calculated based on the known values of $(\underline{H}^{\text{Delay}})_{ijk}^{n-\frac{1}{2}}$, $(\underline{H})_{ijk}^{n+\frac{1}{2}}$ and $(\underline{H})_{ijk}^{n-\frac{1}{2}}$.

(4) Using Eq. (2.40), $(\underline{E})_{ijk}^{n+1}$ is calculated based on the known values of $(\underline{E})_{ijk}^{n}$, $(\underline{E}^{\text{Delay}})_{ijk}^{n}$, $(\underline{Q}_{\rho})_{ijk}^{n}$, $(\underline{Q}_{\rho}^{\text{Delay}})_{ijk}^{n}$ and $(\underline{H})_{ijk}^{n+\frac{1}{2}}$.

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(5) Using Eqs. (2.41), (2.43) and (2.44), $(Q_\rho)_{ijk}^{n+1}$, $(\underline{E}^{Delay})_{ijk}^{n+1}$ and $(Q_\rho^{Delay})_{ijk}^{n+1}$ are calculated based on the known values of $(\underline{E})_{ijk}^{n+1}$, $(\underline{E})_{ijk}^{n}$, $(Q_\rho)_{ijk}^{n}$, $(\underline{E}^{Delay})_{ijk}^{n}$ and $(Q_\rho^{Delay})_{ijk}^{n}$.

(6) Increment the time step by Δt. Go back to step (2) and repeat the whole process over again.

Shown in Figure 1 is the flow chart of numerical steps required to update field values as described above.

In the case of the PML interface to the constant conductivity medium we set $\gamma_\rho = 0$ and α_ρ to be the value of the constant electric conductivity. The result is that the matrix elements simplify to the forms shown in Appendix B. Furthermore, if we set both α_ρ and γ_ρ to zeroes the FDTD-PML algorithm reduces to the case of the simple PML algorithm for the vacuum.

III. CONCLUSIONS

We present in this paper the formulation of a three-dimensional FDTD-PML algorithm inside dispersive PML media that is used to absorb all outgoing electromagnetic waves within a finite simulation volume to create the notion of infinity at the outer layer boundary of the computational volume. Because of the use of the piecewise-linear approximation, the FDTD-PML algorithm provides second-order accuracy in time for the calculation of electromagnetic field quantities inside the outer absorbing layer boundary, resulting in less than one thousandths of the outgoing wave coming back into the main computational volume. Computationally, we can see that the FDTD-PML algorithm retains all the advantages of the usual first-order discrete recursive convolution approach, such as fast computational speed and efficient use of computer memory. In the limit of no PML interface, the FDTD-PML algorithm reduces to a simple FDTD algorithm formulated for linear dispersive media.

Lastly, we need to point out that the exponential form of the susceptibility function is crucial in allowing us to implement the recursive feature in our algorithm.

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This appendix gives the explicit expressions of coefficients and matrices seen in Eqs. (2.39) through (2.44). The coefficients are $\Theta_{\rho,0}$, $\Theta_{\rho,1}$ and $\Theta_{\rho,2}$. The matrices are $\underline{\underline{\Omega_0}}$, $\underline{\underline{\Omega_1}}$, $\underline{\underline{\Omega_2}}$, $\underline{\underline{\Omega_3}}$, $\underline{\underline{\Omega_4}}$, $\underline{\underline{\Omega_5}}$, $\underline{\underline{\Omega_6}}$, $\underline{\underline{\Omega_7}}$, $\underline{\underline{\Omega_8}}$, $\underline{\underline{\Gamma_{\rho,0}}}$, $\underline{\underline{\Pi_{\rho,0}}}$, $\underline{\underline{\Pi_{\rho,1}}}$ and $\underline{\underline{\Pi_{\rho,2}}}$. Also, to express these coefficients and matrices in more compact forms, additional terms, such as $\xi_{\rho,0}$, $\xi_{\rho,1}$, $\xi_{\rho,2}$, $\varsigma_{\rho,1}$, $\varsigma_{\rho,2}$, $(\psi_0)_x$, $(\psi_1)_x$, $(\psi_2)_x$, $(\varphi_1)_x$, $(\varphi_2)_x$, $(\zeta_{\rho,0})_x$, $(\zeta_{\rho,1})_x$, $(\pi_{\rho,0})_x$, $(\pi_{\rho,1})_x$ and $(\pi_{\rho,2})_x$, are defined. These additional terms are shown following the expressions for coefficients and matrices.

$$\Theta_{\rho,0} = \xi_{\rho,0}, \tag{A.1}$$

$$\Theta_{\rho,1} = \frac{\alpha_\rho}{\varepsilon_R}[\xi_{\rho,1} - \xi_{\rho,2}], \tag{A.2}$$

$$\Theta_{\rho,2} = \frac{\alpha_\rho}{\varepsilon_R}\xi_{\rho,2}, \tag{A.3}$$

$$\underline{\underline{\Omega_0}} = \begin{pmatrix} (\Omega_0)_{11} & 0 & 0 \\ 0 & (\Omega_0)_{22} & 0 \\ 0 & 0 & (\Omega_0)_{33} \end{pmatrix} \text{ with three diagonal elements expressed as} \tag{A.4}$$

$$(\Omega_0)_{11} = 1 + [(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) + (\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})]\frac{\Delta t}{2} + [(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})][(\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})](\varphi_2)_x, \tag{A.5}$$

$$(\Omega_0)_{22} = \text{Replace } [x{\to}y, y{\to}z, \text{ and } z{\to}x] \text{ in } (\Omega_0)_{11}, \tag{A.6}$$

$$(\Omega_0)_{33} = \text{Replace } [x{\to}z, y{\to}x, \text{ and } z{\to}y] \text{ in } (\Omega_0)_{11}, \tag{A.7}$$

$$\underline{\underline{\Omega_1}} = \begin{pmatrix} (\Omega_1)_{11} & 0 & 0 \\ 0 & (\Omega_1)_{22} & 0 \\ 0 & 0 & (\Omega_1)_{33} \end{pmatrix} \text{ with three diagonal elements expressed as} \tag{A.8}$$

$$(\Omega_1)_{11} = -1 + [(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) + (\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})]\frac{\Delta t}{2} + [(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})][(\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})][(\varphi_1)_x - (\varphi_2)_x], \tag{A.9}$$

$$(\Omega_1)_{22} = \text{Replace } [x{\to}y, y{\to}z, \text{ and } z{\to}x] \text{ in } (\Omega_1)_{11}, \tag{A.10}$$

$$(\Omega_1)_{33} = \text{Replace } [x{\to}z, y{\to}x, \text{ and } z{\to}y] \text{ in } (\Omega_1)_{11}, \tag{A.11}$$

$$\underline{\underline{\Omega_2}} = \begin{pmatrix} (\Omega_2)_{11} & 0 & 0 \\ 0 & (\Omega_2)_{22} & 0 \\ 0 & 0 & (\Omega_2)_{33} \end{pmatrix} \text{ with three diagonal elements expressed as} \tag{A.12}$$

$$(\Omega_2)_{11} = [(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})][(\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})](\psi_1)_x, \tag{A.13}$$

$$(\Omega_2)_{22} = \text{Replace } [x{\to}y, y{\to}z, \text{ and } z{\to}x] \text{ in } (\Omega_2)_{11}, \tag{A.14}$$

$$(\Omega_2)_{33} = \text{Replace } [x{\to}z, y{\to}x, \text{ and } z{\to}y] \text{ in } (\Omega_2)_{11}, \tag{A.15}$$

$$\underline{\underline{\Omega_3}} = \begin{pmatrix} (\Omega_3)_{11} & 0 & 0 \\ 0 & (\Omega_3)_{22} & 0 \\ 0 & 0 & (\Omega_3)_{33} \end{pmatrix} \text{ with three diagonal elements expressed as} \tag{A.16}$$

$$(\Omega_3)_{11} = 1 + [(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) + (\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\}]\frac{\Delta t}{2} + [(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})][(\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})]\,(\varphi_2)_x$$

$$+\frac{1}{\varepsilon_R}\text{Re}\{\sum_\rho \alpha_\rho \xi_{\rho,0}\xi_{\rho,1}\} + \frac{1}{\varepsilon_R}[(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) + (\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})]\text{Re}\{\sum_\rho \alpha_\rho \varsigma_{\rho,2}\}$$

$$+\frac{1}{\varepsilon_R}[(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})][(\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})]\text{Re}\{\sum_\rho \alpha_\rho (\zeta_{\rho,2})_x\}, \tag{A.17}$$

$$(\Omega_3)_{22} = \text{Replace } [x\rightarrow y, y\rightarrow z, \text{ and } z\rightarrow x] \text{ in } (\Omega_3)_{11}, \tag{A.18}$$

$$(\Omega_3)_{33} = \text{Replace } [x\rightarrow z, y\rightarrow x, \text{ and } z\rightarrow y] \text{ in } (\Omega_3)_{11}, \tag{A.19}$$

$$\underline{\underline{\Omega_4}} = \begin{pmatrix} (\Omega_4)_{11} & 0 & 0 \\ 0 & (\Omega_4)_{22} & 0 \\ 0 & 0 & (\Omega_4)_{33} \end{pmatrix} \text{ with three diagonal elements expressed as} \tag{A.20}$$

$$(\Omega_4)_{11} = -1 + [(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) + (\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})]\frac{\Delta t}{2} + [(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})][(\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})][(\varphi_1)_x - (\varphi_2)_x]$$

$$+\frac{1}{\varepsilon_R}\text{Re}\{\sum_\rho \alpha_\rho \xi_{\rho,0}[\xi_{\rho,1} - \xi_{\rho,2}]\} + \frac{1}{\varepsilon_R}[(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) + (\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})]\text{Re}\{\sum_\rho \alpha_\rho [\varsigma_{\rho,1} - \varsigma_{\rho,2}]\}$$

$$+\frac{1}{\varepsilon_R}[(\frac{\sigma_y}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})][(\frac{\sigma_z}{\varepsilon_0\varepsilon_R}) - (\frac{\sigma_x}{\varepsilon_0\varepsilon_R})]\text{Re}\{\sum_\rho \alpha_\rho [(\zeta_{\rho,1})_x - (\zeta_{\rho,2})_x]\}, \tag{A.21}$$

$$(\Omega_4)_{22} = \text{Replace } [x\rightarrow y, y\rightarrow z, \text{ and } z\rightarrow x] \text{ in } (\Omega_4)_{11}, \tag{A.22}$$

$$(\Omega_4)_{33} = \text{Replace } [x\rightarrow z, y\rightarrow x, \text{ and } z\rightarrow y] \text{ in } (\Omega_4)_{11}, \tag{A.23}$$

$$\underline{\underline{\Omega_5}} = \begin{pmatrix} \frac{1}{\varepsilon_R}(\Omega_2)_{11} & 0 & 0 \\ 0 & \frac{1}{\varepsilon_R}(\Omega_2)_{22} & 0 \\ 0 & 0 & \frac{1}{\varepsilon_R}(\Omega_2)_{33} \end{pmatrix}, \tag{A.24}$$

$$\underline{\underline{\Omega_6}} = \begin{pmatrix} (\psi_0)_x & 0 & 0 \\ 0 & (\psi_0)_y & 0 \\ 0 & 0 & (\psi_0)_z \end{pmatrix}, \tag{A.25}$$

$$\underline{\underline{\Omega_7}} = \begin{pmatrix} [(\psi_1)_x - (\psi_2)_x] & 0 & 0 \\ 0 & [(\psi_1)_y - (\psi_2)_y] & 0 \\ 0 & 0 & [(\psi_1)_z - (\psi_2)_z] \end{pmatrix}, \tag{A.26}$$

$$\underline{\underline{\Omega_8}} = \begin{pmatrix} (\psi_2)_x & 0 & 0 \\ 0 & (\psi_2)_y & 0 \\ 0 & 0 & (\psi_2)_z \end{pmatrix}, \tag{A.27}$$

$$\underline{\underline{\Gamma_{\rho,0}}} = \begin{pmatrix} (\Gamma_{\rho,0})_{11} & 0 & 0 \\ 0 & (\Gamma_{\rho,0})_{22} & 0 \\ 0 & 0 & (\Gamma_{\rho,0})_{33} \end{pmatrix} \text{ with three diagonal elements expressed as} \tag{A.28}$$

$$(\Gamma_{\rho,0})_{11} = [\,\xi_{\rho,0} - 1\,] + [\,(\frac{\sigma_y}{\epsilon_0\epsilon_R}) + (\frac{\sigma_z}{\epsilon_0\epsilon_R}) - (\frac{\sigma_x}{\epsilon_0\epsilon_R})\,]\,\xi_{\rho,1}$$

$$+ [(\frac{\sigma_y}{\epsilon_0\epsilon_R}) - (\frac{\sigma_x}{\epsilon_0\epsilon_R})][(\frac{\sigma_z}{\epsilon_0\epsilon_R}) - (\frac{\sigma_x}{\epsilon_0\epsilon_R})]\,(\zeta_{\rho,0})_x\,, \tag{A.29}$$

$$(\Gamma_{\rho,0})_{22} = \text{Replace } [x\rightarrow y,\ y\rightarrow z,\ \text{and } z\rightarrow x]\ \text{in}\ (\Gamma_{\rho,0})_{11}\,, \tag{A.30}$$

$$(\Gamma_{\rho,0})_{33} = \text{Replace } [x\rightarrow z,\ y\rightarrow x,\ \text{and } z\rightarrow y]\ \text{in}\ (\Gamma_{\rho,0})_{11}\,, \tag{A.31}$$

$$\underline{\underline{\Pi_{\rho,0}}} = \begin{pmatrix} \frac{\alpha_\rho}{\epsilon_R}(\pi_{\rho,0})_x & 0 & 0 \\[2mm] 0 & \frac{\alpha_\rho}{\epsilon_R}(\pi_{\rho,0})_y & 0 \\[2mm] 0 & 0 & \frac{\alpha_\rho}{\epsilon_R}(\pi_{\rho,0})_z \end{pmatrix}, \tag{A.32}$$

$$\underline{\underline{\Pi_{\rho,1}}} = \begin{pmatrix} \frac{\alpha_\rho}{\epsilon_R}[(\pi_{\rho,1})_x - (\pi_{\rho,2})_x] & 0 & 0 \\[2mm] 0 & \frac{\alpha_\rho}{\epsilon_R}[(\pi_{\rho,1})_y - (\pi_{\rho,2})_y] & 0 \\[2mm] 0 & 0 & \frac{\alpha_\rho}{\epsilon_R}[(\pi_{\rho,1})_z - (\pi_{\rho,2})_z] \end{pmatrix}, \tag{A.33}$$

$$\underline{\underline{\Pi_{\rho,2}}} = \begin{pmatrix} \frac{\alpha_\rho}{\epsilon_R}(\pi_{\rho,2})_x & 0 & 0 \\[2mm] 0 & \frac{\alpha_\rho}{\epsilon_R}(\pi_{\rho,2})_y & 0 \\[2mm] 0 & 0 & \frac{\alpha_\rho}{\epsilon_R}(\pi_{\rho,2})_z \end{pmatrix}, \tag{A.34}$$

and matrix elements are defined as follows

$$\xi_{\rho,0} \equiv \exp[-(\gamma_\rho)\Delta t]\,, \tag{A.35}$$

$$\xi_{\rho,1} \equiv \int_0^{\Delta t} d\tau\, \exp[-(\gamma_\rho)\tau] = \Delta t\,\Big[\frac{1 - \exp[-(\gamma_\rho)\Delta t]}{(\gamma_\rho)\Delta t}\Big]\,, \tag{A.36}$$

$$\xi_{\rho,2} \equiv \int_0^{\Delta t} d\tau\,(\frac{\tau}{\Delta t})\,\exp[-(\gamma_\rho)\tau] = \Delta t\,\frac{1}{(\gamma_\rho)\Delta t}\Big[\frac{1 - \exp[-(\gamma_\rho)\Delta t]}{(\gamma_\rho)\Delta t} - \exp[-(\gamma_\rho)\Delta t]\Big]\,, \tag{A.37}$$

$$\varsigma_{\rho,1} \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau'\exp[-(\gamma_\rho)(\tau - \tau')] = (\Delta t)^2\,\frac{1}{(\gamma_\rho)\Delta t}\Big[1 - \frac{1 - \exp[-(\gamma_\rho)\Delta t]}{(\gamma_\rho)\Delta t}\Big]\,, \tag{A.38}$$

$$\varsigma_{\rho,2} \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau'\,(\frac{\tau}{\Delta t})\,\exp[-(\gamma_\rho)(\tau - \tau')]$$

$$= (\Delta t)^2\,\frac{1}{(\gamma_\rho)\Delta t}\Big[\frac{1}{2} - \frac{1}{(\gamma_\rho)\Delta t}\Big[1 - \frac{1 - \exp[-(\gamma_\rho)\Delta t]}{(\gamma_\rho)\Delta t}\Big]\Big]\,, \tag{A.39}$$

For the x component:

$$(\psi_0)_x \equiv \exp[-(\frac{\sigma_x}{\epsilon_0\epsilon_R})\Delta t]\,, \tag{A.40}$$

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$$(\psi_1)_x \equiv \int_0^{\Delta t} d\tau \exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\tau] = \Delta t \left[\frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right], \tag{A.41}$$

$$(\psi_2)_x \equiv \int_0^{\Delta t} d\tau (\frac{\tau}{\Delta t}) \exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\tau] = \Delta t \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[\frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} - \exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]] \right], \tag{A.42}$$

$$(\varphi_1)_x \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau' \exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})(\tau-\tau')] = (\Delta t)^2 \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right], \tag{A.43}$$

$$(\varphi_2)_x \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau' (\frac{\tau'}{\Delta t}) \exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})(\tau-\tau')]$$

$$= (\Delta t)^2 \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[\frac{1}{2} - \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \right], \tag{A.44}$$

$$(\zeta_{\rho,0})_x \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau' \exp[-(\gamma_\rho)\tau'] \exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})(\tau-\tau')]$$

$$= (\Delta t)^2 \frac{1}{[(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t - (\gamma_\rho)\Delta t]} \left[\frac{1-\exp[-(\gamma_\rho)\Delta t]}{(\gamma_\rho)\Delta t} - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right], \tag{A.45}$$

$$(\zeta_{\rho,1})_x \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau' \int_0^{\tau'} d\tau'' \exp[-(\gamma_\rho)(\tau'-\tau'')] \exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})(\tau-\tau')]$$

$$= (\Delta t)^3 \frac{1}{(\gamma_\rho)\Delta t} \left\{ \left[\frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \right.$$

$$\left. - \left[\frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t - (\gamma_\rho)\Delta t} \right] \left[\frac{1-\exp[-(\gamma_\rho)\Delta t]}{(\gamma_\rho)\Delta t} - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \right\}, \tag{A.46}$$

$$(\zeta_{\rho,2})_x \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau' \int_0^{\tau'} d\tau'' (\frac{\tau''}{\Delta t}) \exp[-(\gamma_\rho)(\tau'-\tau'')] \exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})(\tau-\tau')]$$

$$= (\Delta t)^3 \frac{1}{(\gamma_\rho)\Delta t} \left\{ \left[\frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \left[\frac{1}{2} - \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \left[\frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} + \frac{1}{(\gamma_\rho)\Delta t} \right] \right] \right.$$

$$\left. + \left[\frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t - (\gamma_\rho)\Delta t} \right] \left[\frac{1}{(\gamma_\rho)\Delta t} \right] \left[\frac{1-\exp[-(\gamma_\rho)\Delta t]}{(\gamma_\rho)\Delta t} - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \right\}, \tag{A.47}$$

$$(\pi_{\rho,0})_x \equiv \int_0^{\Delta t} d\tau \, \exp[-(\gamma_\rho)\tau]\exp[(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\tau]$$

$$= \Delta t \exp[(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]\left[\frac{\exp[-(\gamma_\rho)\Delta t]-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t-(\gamma_\rho)\Delta t}\right], \qquad (A.48)$$

$$(\pi_{\rho,1})_x \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau' \exp[-(\gamma_\rho)(\tau-\tau')] \exp[(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\tau]$$

$$= (\Delta t)^2 \frac{\exp[(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\gamma_\rho)\Delta t}\left\{ \left[\frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t}\right] - \left[\frac{\exp[-(\gamma_\rho)\Delta t]-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]-}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t-(\gamma_\rho)\Delta t}\right]\right\}, \quad (A.49)$$

$$(\pi_{\rho,2})_x \equiv \int_0^{\Delta t} d\tau \int_0^{\tau} d\tau'(\frac{\tau'}{\Delta t}) \exp[-(\gamma_\rho)(\tau-\tau')] \exp[(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\tau]$$

$$= (\Delta t)^2 \frac{\exp[(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{[(\gamma_\rho)\Delta t][(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}\left\{ 1-\left[\frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t}\right]\left[1+\frac{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta}{(\gamma_\rho)\Delta t}\right]\right.$$

$$\left. -\left[\frac{\exp[-(\gamma_\rho)\Delta t]-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t-(\gamma_\rho)\Delta t}\right]\left[\frac{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t}{(\gamma_\rho)\Delta t}\right]\right\}, \qquad (A.50)$$

For the y component:
Replace [x→y] of matrix elements defined for the x component above.
For the z component:
Replace [x→z] of matrix elements defined for the x component above.

As noted in the definition of matrix elements above, these elements depend only on known values Δt, α_ρ, γ_ρ, σ_x, σ_y and σ_z.

APPENDIX B

By letting $\gamma_\rho \to 0$ in Eqs. (A.35) through (A.50) we can obtain the following matrix elements for the case of the constant conductivity.

$$\xi_{\rho,0} = 1, \qquad (B.1)$$

$$\xi_{\rho,1} = \Delta t, \qquad (B.2)$$

$$\xi_{\rho,2} = \frac{\Delta t}{2}, \qquad (B.3)$$

$$\varsigma_{\rho,1} = \frac{(\Delta t)^2}{2}, \qquad (B.4)$$

$$\varsigma_{\rho,2} = \frac{(\Delta t)^2}{6} \qquad (B.5)$$

For the x component:

$$(\psi_0)_x = \exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t] , \tag{B.6}$$

$$(\psi_1)_x = \Delta t \left[\frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] , \tag{B.7}$$

$$(\psi_2)_x = \Delta t \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t)]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] , \tag{B.8}$$

$$(\varphi_1)_x = (\Delta t)^2 \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] , \tag{B.9}$$

$$(\varphi_2)_x = (\Delta t)^2 \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[\frac{1}{2} - \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \right] , \tag{B.10}$$

$$(\zeta_{\rho,0})_x = (\Delta t)^2 \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] , \tag{B.11}$$

$$(\zeta_{\rho,1})_x = (\Delta t)^2 \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[\frac{1}{2} - \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \right] , \tag{B.12}$$

$$(\zeta_{\rho,2})_x = (\Delta t)^3 \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left\{ \frac{1}{6} - \left[\frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[\frac{1}{2} - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \right] \right\} , \tag{B.13}$$

$$(\pi_{\rho,0})_x = \Delta t \left[\frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] , \tag{B.14}$$

$$(\pi_{\rho,1})_x = (\Delta t)^2 \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] , \tag{B.15}$$

$$(\pi_{\rho,2})_x = (\Delta t)^2 \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[\frac{1}{2} - \frac{1}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \left[1 - \frac{1-\exp[-(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t]}{(\frac{\sigma_x}{\varepsilon_0\varepsilon_R})\Delta t} \right] \right] , \tag{B.16}$$

For the y component:
    Replace [x→y] of matrix elements defined for the x component above,
For the z component:
    Replace [x→z] of matrix elements defined for the x component above.

Flow Chart

Calculate $(\underline{H})_{ijk}{}^{n+\frac{1}{2}}$

Calculate $(\underline{H}^{Delay})_{ijk}{}^{n+\frac{1}{2}}$

Calculate $(\underline{E})_{ijk}{}^{n+1}$

Calculate $(Q_{\rho}{}^{L})_{ijk}{}^{n+1}$, $(\underline{E}^{Delay})_{ijk}{}^{n+1}$, and $(\underline{Q}_{\rho}{}^{Delay})_{ijk}{}^{n+1}$

Increment to the next time step

Reached the maximum time ?

No

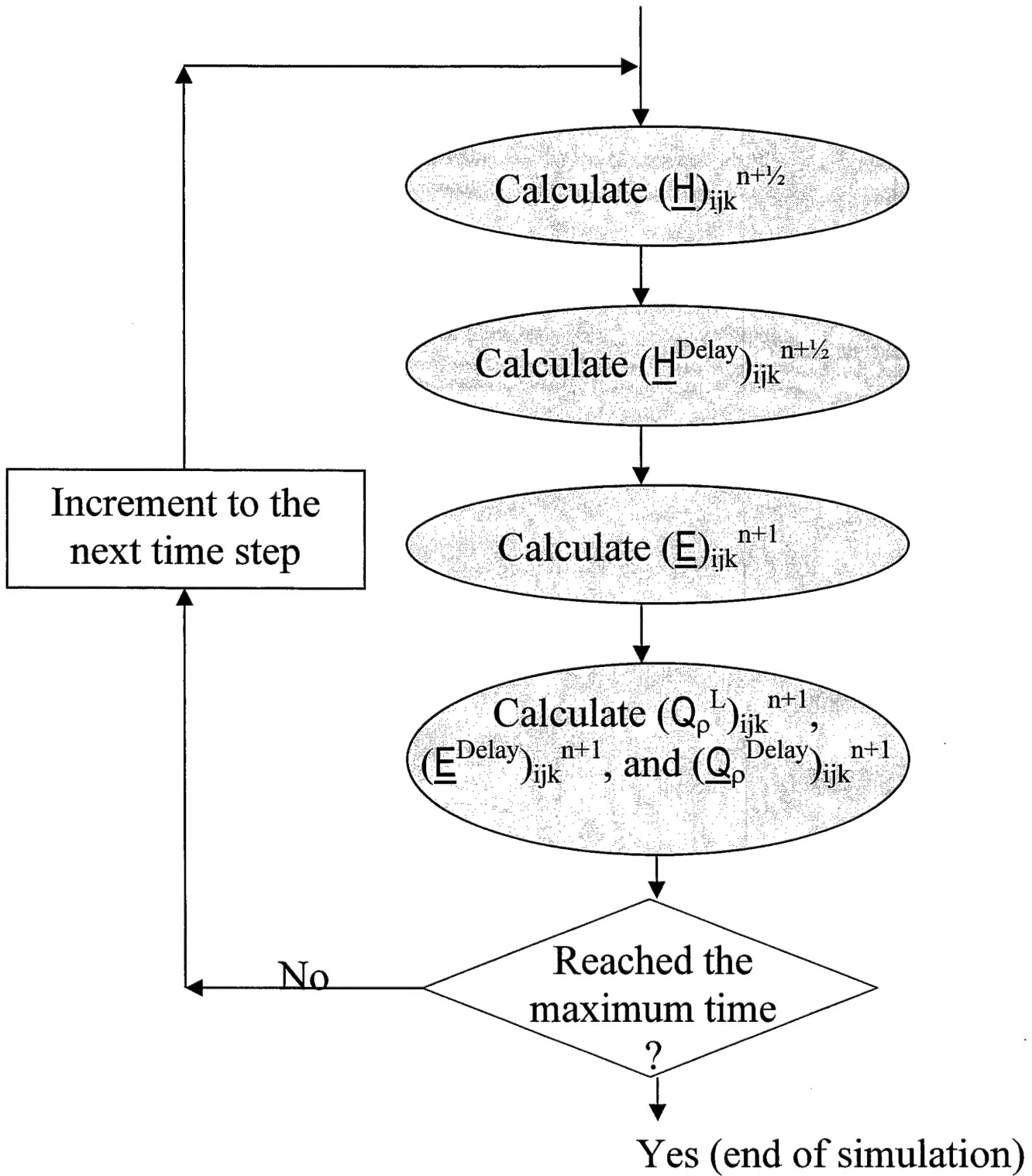Yes (end of simulation)

Figure 1: Flow chart of the dispersive FDTD-PML algorithm

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